

Multi-step Bose-Einstein Condensation of Trapped Ideal Bose Gases

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Abstract: The Phenomenon of multi-step Bose-Einstein condensation (BEC) of a finite number of non-interacting bosons in anisotropic traps has been demonstrated by studying the populations on eight subsets of states. The cusp in the specific heat is found to be associated with the crossover between subsets of states involving Bose functions $g_n(z)$ of different classes, as specified by their behaviour at $z = 1$.

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1. Introduction

The experimental realizations [1] of Bose-Einstein condensation (BEC) [2] in trapped dilute alkali atomic vapours have attracted much attention recently. Standard textbooks [3] on statistical mechanics typically treats the topics of non-interacting free Bose gas in one, two, and three dimensional boxes in the thermodynamic limit. BEC is defined as the onset of a macroscopic occupation of the ground state at a finite temperature, and it is usually accompanied by a cusp in the temperature dependence of the specific heat [3,4].

Recent theoretical studies on BEC have revealed interesting effects of finite number of particles and anisotropic traps [5–18]. van Druten and Ketterle [6] introduced the concept of two-step BEC to explain the observation that the cusp in the specific heat appears at a temperature T_{cusp} significantly higher than the BEC critical temperature T_c in anisotropic harmonic traps. This phenomena comes about from the changes in the occupations of states in the anisotropic trap with different characters as the temperature is lowered. In the present work, we study the intermediate steps towards BEC in details. We introduce the concept of dividing the set of all single particle states into eight subsets, each of which consisting of states with different characters. Such a division is especially useful in treating particles in anisotropic traps in that the states in the subsets can be classified into those corresponding to zero-point motion, excited states of oscillators in one, two, and three dimensions. The occupations in these subsets can be evaluated numerically or by invoking a continuum approximation using the concept of the density of states. The possible multi-step phenomena associated with BEC can then be described in terms of the changes in the relative populations in the different subsets as the temperature is lowered. We found that phenomena involving more than two steps can occur in a general class of highly anisotropic traps. We also found that two-step BEC is possible in anisotropic traps with $\omega_1 = \omega_2 \ll \omega_3$, in contrast to previous claims [6]. The position of the cusp in the specific heat can also be studied within the context of subsets of states. The occupations in the subsets, within the continuum approximation, can be expressed in terms of Bose functions $g_n(z)$. The Bose functions can be classified into two classes according to their behaviour at $z = 1$. Our

results indicate that the cusp in the specific heat appears in the vicinity of the crossovers in the populations between subsets of states involving Bose functions in *different classes* as temperature decreases.

The plan of the paper is as follows. The eight subsets of states are introduced in Sec.2 together with the method of numerical calculations. Section 3 gives a short discussion on the density of states within the continuum approximation. In Sec.4, we present our results demonstrating the possibility of multi-step phenomena towards BEC in anisotropic harmonic traps. Section 5 gives a discussion on the cusp in the specific heat in terms of the crossover between populations in subsets involving Bose functions of different classes. A brief summary is given in Sec.6.

2. Eight subsets of single-particle states

We consider non-interacting bosons trapped in a three-dimensional (3D) anisotropic harmonic traps described by the characteristic frequencies ω_1 , ω_2 , and ω_3 in the \hat{x} , \hat{y} , and \hat{z} -axis. The single particle energy spectrum can be characterized by the quantum numbers n_1 , n_2 , and n_3 . To facilitate our discussion, we divide the set $S = \{(n_1, n_2, n_3) : n_1, n_2, n_3 = 0, 1, 2, \dots\}$ of all single particle states into eight subsets with different properties, i.e., $S = S_0 \oplus S_1 \oplus S_2 \oplus S_3 \oplus S_{12} \oplus S_{13} \oplus S_{23} \oplus S_{123}$. Here $S_0 = \{(0, 0, 0)\}$ consists only of the overall ground state. The subsets $S_1 = \{(n_1, 0, 0) : n_1 = 1, 2, \dots\}$, $S_2 = \{(0, n_2, 0) : n_2 = 1, 2, \dots\}$, and $S_3 = \{(0, 0, n_3) : n_3 = 1, 2, \dots\}$ consist of states in which the lowest energy state of the corresponding harmonic oscillators in two of the three spatial directions are occupied and the excited states in only one spatial dimension are occupied. Hence, S_1 , S_2 , and S_3 include states which are one dimensional (1D) in character. Similarly, the subsets S_{12} , S_{13} , and S_{23} consist of states which are two dimensional (2D) in character in that they consist of states in which one and only one of the three quantum numbers vanishes, and hence include states which are excited in the xy , xz , and yz planes, respectively. The subset $S_{123} = \{(n_1, n_2, n_3) : n_1, n_2, n_3 = 1, 2, \dots\}$ consists of all the 3D excited states with nonzero n_1 , n_2 , and n_3 .

The mean occupation number n_p in a single-particle state with energy ϵ_p is given, within

the grand-canonical ensemble, by

$$n_p = \frac{1}{e^{\beta(\epsilon_p - \mu)} - 1}, \quad (1)$$

where $\beta \equiv 1/k_B T$ is the inverse temperature with k_B being the Boltzmann constant. The chemical potential μ or the fugacity $z \equiv \exp(\beta\mu)$ is determined by the mean number of particles N in the system via $N = \sum_p n_p$. Defining [17] the factor $B_j \equiv \sum_p \exp(-j\beta\epsilon_p)$, where the summation is over all the single-particle states labelled by p , then we have

$$N = \sum_{j=1}^{\infty} z^j B_j. \quad (2)$$

Note that all the effects of the confining potential on the thermodynamic properties are included in the factor B_j through the energy spectrum ϵ_p . For the 3D parabolic potential with possibly different frequencies in different directions, the single-particle eigen-energies are given by $\epsilon_{n_i} = \sum_{i=1}^3 n_i \hbar \omega_i$, where $\omega_1 \leq \omega_2 \leq \omega_3$ are the frequencies characterizing the confinement in different directions. The quantum numbers n_1 , n_2 , and n_3 take on non-negative integers, and the zero-point energy has been absorbed into the definition of the zero of energy. Once the fugacity z is determined by Eq.(2), the internal energy U can be calculated directly via $U = -\sum_{j=1}^{\infty} z^j (\partial B_j / \partial \beta) / j$, and the heat capacity $C_v = (\partial U / \partial T)_{N,v}$ can also be obtained. The subscript v in C_v indicates that this quantity is analogous to the heat capacity at fixed volume in the sense that the oscillators' frequencies are held fixed. The occupation in each of the subsets of states can also be evaluated as a function of temperature. Equation (2) forms the basis of our discussion of multi-step phenomena associated with BEC.

3. Continuum approximation using DOS

In addition to studying the mean occupation in each subset of states numerically, we can also study the occupations analytically by invoking the notion of the density of states (DOS) [3,4,6–11]. The DOS for each of the subsets can readily be written down. However, one should keep in mind the fact that the different subsets of states have *different* lower limits of energy when a sum over states is turned into an integral, a point that has become

a source of confusion in the literature [4,7]. The mean occupation numbers in the eight subsets of states can then be expressed as:

$$\begin{cases} N_0 & \approx g_0(z), \\ N_i & \approx \frac{1}{\Omega_i} g_1(z e^{-\Omega_i^*}), \quad i = 1, 2, 3, \\ N_{i\ell} & \approx \frac{1}{\Omega_i \Omega_\ell} g_2(z e^{-\Omega_\ell^*}), \quad \ell = 12, 13, 23, \\ N_{123} & \approx \frac{1}{\Omega_1 \Omega_2 \Omega_3} g_3(z e^{-\Omega_{123}^*}). \end{cases} \quad (3)$$

Here $\Omega_i \equiv \hbar\omega_i/k_B T$ ($i = 1, 2, 3$), $\Omega^* \equiv \epsilon^*/k_B T$, and the proper lower limits of energy for integrations involving the DOS for subsets corresponding to excited states with 1D, 2D, and 3D characters should be taken to be $\epsilon_i^* = \hbar\omega_i/2$ ($i = 1, 2, 3$), $\epsilon_{i\ell}^* = \hbar(\omega_i + \omega_\ell)/2$ ($i\ell = 12, 13, 23$), and $\epsilon_{123}^* = \hbar(\omega_1 + \omega_2 + \omega_3 + \sqrt{\omega_1^2 + \omega_2^2 + \omega_3^2})/2$, respectively. The Bose functions $g_n(z)$ are defined [3] by $g_n(z) = \sum_{j=1}^{\infty} z^j/j^n$. These functions can be divided into *two classes*. The first class consists of Bose functions with $n > 1$, and they are finite at $z = 1$. The second class consists of Bose functions with $n \leq 1$, and they diverge at $z = 1$. For example, $g_0(z) = z/(1 - z)$ and $g_1(z) = -\ln(1 - z)$ diverge at $z = 1$. The results in Eq.(3) also give us insight into the multi-step phenomena associated with BEC as the dominant subset of states carrying a substantial fraction of the total particles changes from one subset to another as the temperature is lowered. Similar approximate expressions for the DOS can be obtained in various different ways such as the Euler-Maclaurin summation [8], the zeta function [10,19], or the simple series [6]. In the approximation scheme of Ref. [6], the single-particle states are divided into four groups.

4. Multi-step BEC

BEC is usually described as the onset of a macroscopic occupation of the overall ground state, i.e., the subset S_0 , at the critical temperature T_c . Very often, it is accompanied by the presence of a cusp in the specific heat at the same temperature. In recent experiments [1,5], the direct evidence for BEC is taken to be the abrupt increase in the peak density at the center of the trapped atomic cloud. Novel experimental techniques have made possible the measurements in the spatial and velocity distributions of the trapped bosons. If the subset of states containing the largest fraction of particles changes from one subset to another

consisting of states with a lower dimensional character as temperature decreases, the changes in the spatial and velocity distributions should also be measurable. In fact, these changes in the characteristic of the trapped bosons have been taken to be the indication of two-step phenomena in BEC [6,7]. Here we will study the possible multi-step phenomena in BEC due to the changes in the occupations in the subsets of states as temperature decreases [19].

Following Ref.[6], a “saturation” temperature can be defined for each subset of excited states. Consider a hypothetical system consisting only of one subset of states, say S_{123} , plus the overall ground state. At the saturation temperature $T_{3D}^{(0)}$, the population in the set of excited states saturates. From Eq.(3), $T_{3D}^{(0)}$ is approximately given by $T_{3D}^{(0)} = (0.94\hbar/k_B)(N\omega_1\omega_2\omega_3)^{1/3}$. Similarly, the “saturation” temperature for the subsets S_{ij} ($ij = 12, 13, 23$) with 2D character is given by $T_{2D}^{(0)} = (0.78\hbar/k_B)(N\omega_i\omega_j)^{1/2}$; and that for the subsets S_i ($i = 1, 2, 3$) of 1D character is given by $T_{1D}^{(0)} \approx (N\hbar\omega_i/k_B) \ln(2N)$ [6,7]. For example, only the subsets S_{123} and S_0 are responsible for the BEC in 3D *isotropic* harmonic trap, and the “saturate temperature” $T_{3D}^{(0)} = 0.94N^{1/3}\hbar\omega/k_B$ is the corresponding critical temperature below which the overall ground state becomes macroscopically occupied.

For suitably chosen ω_1 , ω_2 , and ω_3 , the competitions among the different subsets may lead to complicated and interesting phenomena. Consider $\omega_3 : \omega_2 : \omega_1 = 2.1 \times 10^4 : 4.4 \times 10^3 : 1$. This choice of parameters corresponds to $T_{3D}^{(0)} = 1.21T_{2D}^{(0)}$ and $T_{2D}^{(0)} = 2T_{1D}^{(0)}$. Figure 1 shows the typical behavior of three-step phenomena associated with BEC for $N = 10^5$ particles in such anisotropic traps. The temperature is expressed in reduced temperature defined by $\tau \equiv k_B T / (\hbar^3 \omega_1 \omega_2 \omega_3)^{1/3}$. As the temperature is lowered, the subset containing the largest fraction of particles changes from S_{123} to S_{12} at about $\tau_1 = 1.5$ (the first step), then from S_{12} to S_1 at $\tau_2 = 0.6$ (the second step), and finally to S_0 at about $\tau_3 = 0.2$ (the third step). On the other hand, the BEC critical temperature at which N_0 becomes appreciable is at about $\tau_c = 0.5$. Figure 1 also shows the behavior of the heat capacity. The cusp in the heat capacity appears at $\tau_{cusp} = 0.65$, which is higher than τ_c .

Figure 2 shows the results for $N = 10^5$ bosons in an anisotropic trap with $\omega_1 = \omega_2 = \omega_3/500$. It was reported in Ref. [6] that two-step phenomena will not be observed in such

system since τ_{cusp} and τ_c are nearly the same ($\tau_{cusp} \approx \tau_c = 0.65$). The choice of parameters corresponds to the case in which $\omega_1 = \omega_2 \ll \omega_3$, and we have $T_{3D}^{(0)}/T_{2D}^{(0)} = 1.21(\omega_3^2/\omega_1^2 N)^{1/6} \approx 1.41$. However, our results demonstrated that the particles start to condense from the subset S_{123} into S_{12} at a temperature $\tau_1 \approx 2.0$, and then to S_0 at a lower temperature. Such two-step phenomena should be observable.

5. Cusp in specific heat and crossover between subsets

Our approach of focusing on the occupation in the subsets of states also shed light on the position of the cusp in the heat capacity. In the standard textbook case of ideal Bose gas in the thermodynamical limit, the temperature T_{cusp} corresponding to the position of the cusp coincides with the critical temperature T_c of BEC. However, there exists in general no such restrictions requiring the coincidence of the two temperatures for systems with finite number of particles in anisotropic traps [6]. Recall that the Bose functions $g_n(z)$ can be classified into two classes depending on their behavior at $z = 1$. For harmonic traps, the occupations in S_{123} , S_{12} , S_{13} , S_{23} involve $g_n(z)$ with $n > 1$ (the first class) while the occupations in the subsets S_0 , S_1 , S_2 , S_3 involve $g_n(z)$ with $n \leq 1$ (the second class). An interesting question is that whether there will exist two or more cusps in the specific heat in multi-step phenomena associated with BEC. We have studied the temperature dependence of the specific heat for a wide range of ratios of ω_1 , ω_2 , and ω_3 . Our results indicate that there is at most one peak in the temperature dependence of the heat capacity, with the peak being rounded off due to the finite number of particles in our calculations. The position T_{cusp} of the cusp appears to be the results of a combination of crossovers in the occupations between subsets involving $g_n(z)$ belonging to the two *different classes*. The crossovers at which the particles condense from one subset to another involving Bose functions belonging to the same class do not lead to a cusp in the specific heat. For the system considered in Fig.1, one such crossover occurs between the subsets S_{123} and S_1 at $\tau \approx 0.85$, which coincides with a rapid increase in the heat capacity as temperature decreases. Another crossover between the subsets S_{12} and S_1 at $\tau = 0.65$ coincides with the cusp in the heat capacity. For the case in Fig.2, the crossover between the two classes of Bose functions occurs between the subsets S_{123} and S_0 at $\tau \sim 0.65$,

which coincides with the position of the cusp in the heat capacity. We further re-examine the case of 10^6 bosons in a highly anisotropic trap with $\omega_2 = \omega_3 = 5.6 \times 10^6 \omega_1$ corresponding to $T_{3D}^{(0)} = 2T_{2D}^{(0)}$. This system was studied in Ref. [6] to demonstrate the two-step phenomena. Results are shown in Fig.3. The critical temperature T_c is appreciably lower than T_{cusp} . The position of the cusp coincides with the range of temperatures in which the two crossovers, one between (S_{12}, S_{13}) and S_1 , and another between S_{123} and S_1 , involving different classes of Bose functions occur.

It should be pointed out that our analysis reproduces the standard results in isotropic traps. For isotropic harmonic traps in 3D (2D), BEC is accompanied by a crossover in occupations between S_{123} (S_{12}) and S_0 and hence $T_{cusp} = T_c$ as S_{123} (S_{12}) and S_0 involve different classes of $g_n(z)$. For 1D harmonic traps, BEC is accompanied by the crossover between S_0 and S_1 , both of which involve Bose functions of the same class and hence there exists no cusp in the heat capacity.

Extending our argument to bosons in 3D boxes with dimensions L_1, L_2 and L_3 in different directions is interesting [6]. The occupation in a subset of states with d -dimensional character involves the Bose function $g_{d/2}$ [3]. Hence only the subset S_{123} including excited states in all three Cartesian coordinates involves $g_n(z)$ with $n = 3/2 > 1$. All the other subsets consist of states of lower-dimensional characters and involve $g_n(z)$ with $n \leq 1$. Thus, BEC occurs as long as the spatial dimensions of the box and the number of particles allow the subset S_{123} to be occupied. For a box with $L_1 \ll L_2 \ll L_3$, we expect a three-step BEC to occur with the largest occupation changes, as temperature decreases, from S_{123} to S_{23} , then to S_3 , and finally to S_0 with the cusp of the specific heat appearing in the vicinity of the crossover between S_{123} and S_{23} . The crossover from S_{23} to S_3 and from S_3 to S_0 do not lead to a cusp in the specific heat since the subsets involve Bose functions belonging to the same class. For a box with $L_1 \ll L_2 = L_3$, we expect a two-step phenomena with the cusp of the specific heat appearing at a temperature near the crossover between the subsets S_{123} and S_{23} which is higher than the BEC critical temperature. For a box with $L_1 = L_2 \ll L_3$, we expect that the cusp to appear when near the crossover between S_{123} and S_3 at a temperature higher

than the BEC temperature.

6. Summary

In summary, we have studied the intermediate steps towards BEC for finite number of bosons confined by anisotropic harmonic traps. Using the concept of dividing the set of all single particle states into subsets consisting of states with different characters, two-step and multi-step phenomena associated with BEC can be described in terms of the crossovers in the populations of these subsets as temperature is lowered. Cases with three-step processes are demonstrated. The cusp of the specific heat is found to be associated with the crossover between subsets involving Bose functions of different classes. The general method adopted in the present work can readily be extended to study bosons in other types of traps.

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FIGURES

FIG. 1. Numerical results for $N = 10^5$ particles in a 3D anisotropic harmonic trap with $\omega_3 : \omega_2 : \omega_1 = 2.1 \times 10^4 : 4.4 \times 10^3 : 1$. The solid lines show the temperature dependence of the populations N_0/N in the subset S_0 , N_1/N , N_{12}/N , and N_{123}/N in the subsets S_1 , S_{12} and S_{123} , respectively. The populations in the other subsets are too small to be shown. The line with circles gives the rescaled specific heat as a function of the reduced temperature $\tau \equiv k_B T / (\hbar^3 \omega_1 \omega_2 \omega_3)^{1/3}$.

FIG. 2. Two-step BEC occurs in a Bose gas of $N = 10^5$ particles in an anisotropic trap with $\omega_3 : \omega_2 : \omega_1 = 500 : 1 : 1$. The particles condense from the subset S_{123} into the subset S_{12} at a temperature significantly higher than the BEC critical temperature, showing features of a two-step BEC. However, the temperature for specific heat cusp is close to the BEC critical temperature.

FIG. 3. Typical behaviour of two-step BEC of $N = 10^6$ particles in a highly anisotropic harmonic trap with $\omega_3 = \omega_2 = 5.6 \times 10^6 \omega_1$, corresponding to $T_{3D}^{(0)} = 2T_{1D}^{(0)}$. The condensations from the subsets S_{123} , S_{12} , and S_{13} to S_1 are responsible for the cusp in the specific heat.

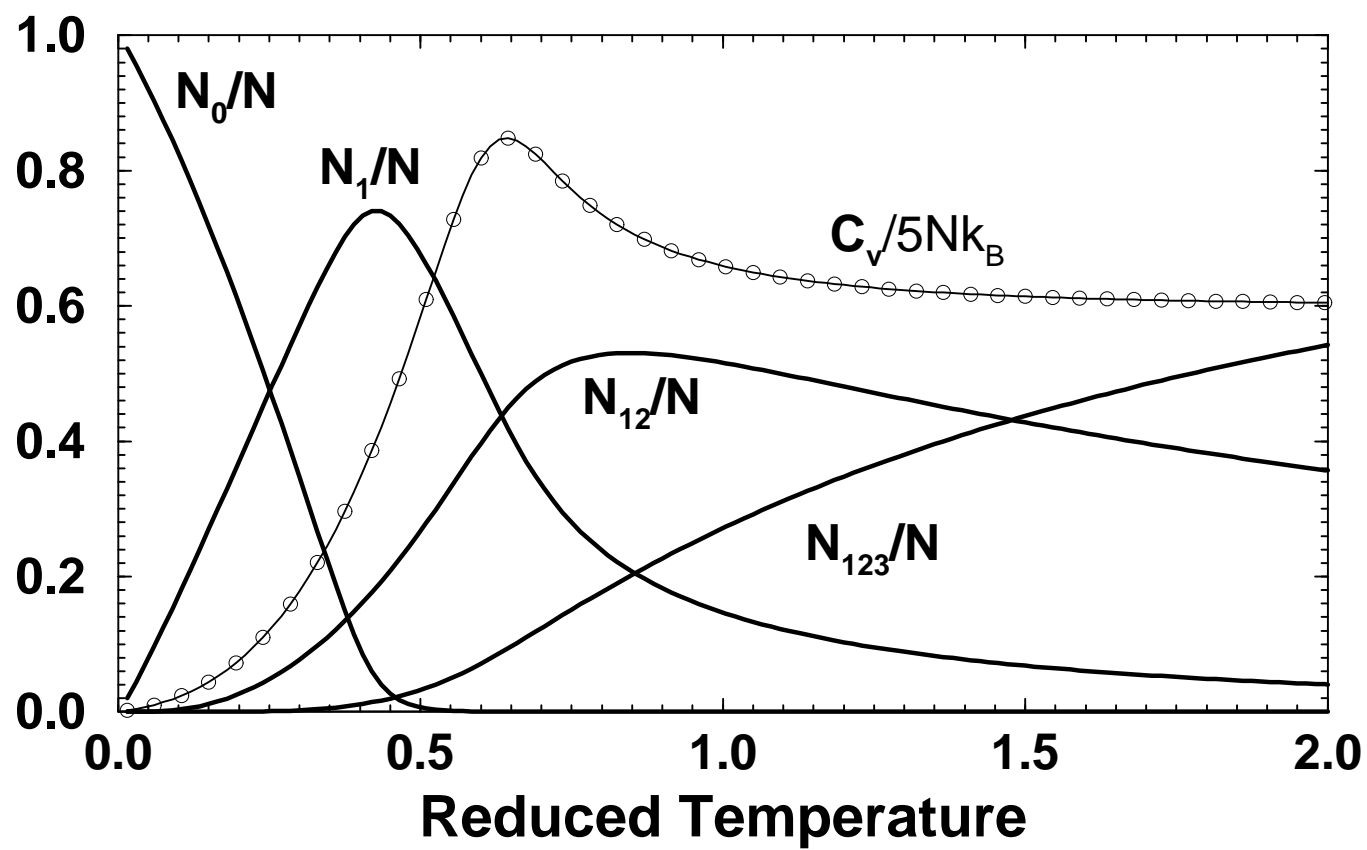


Fig.1 Wenji DENG

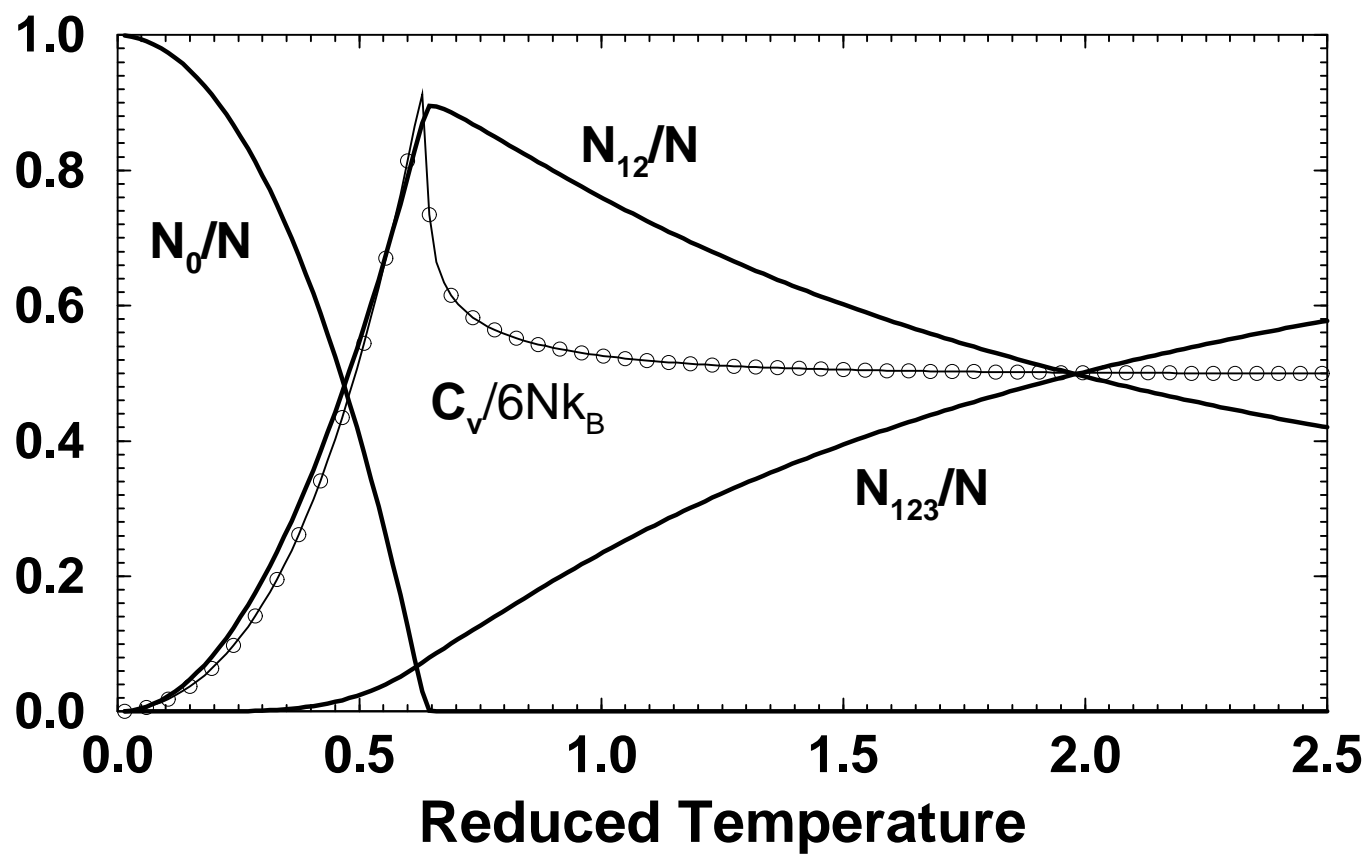


Fig.2 Wenji DENG

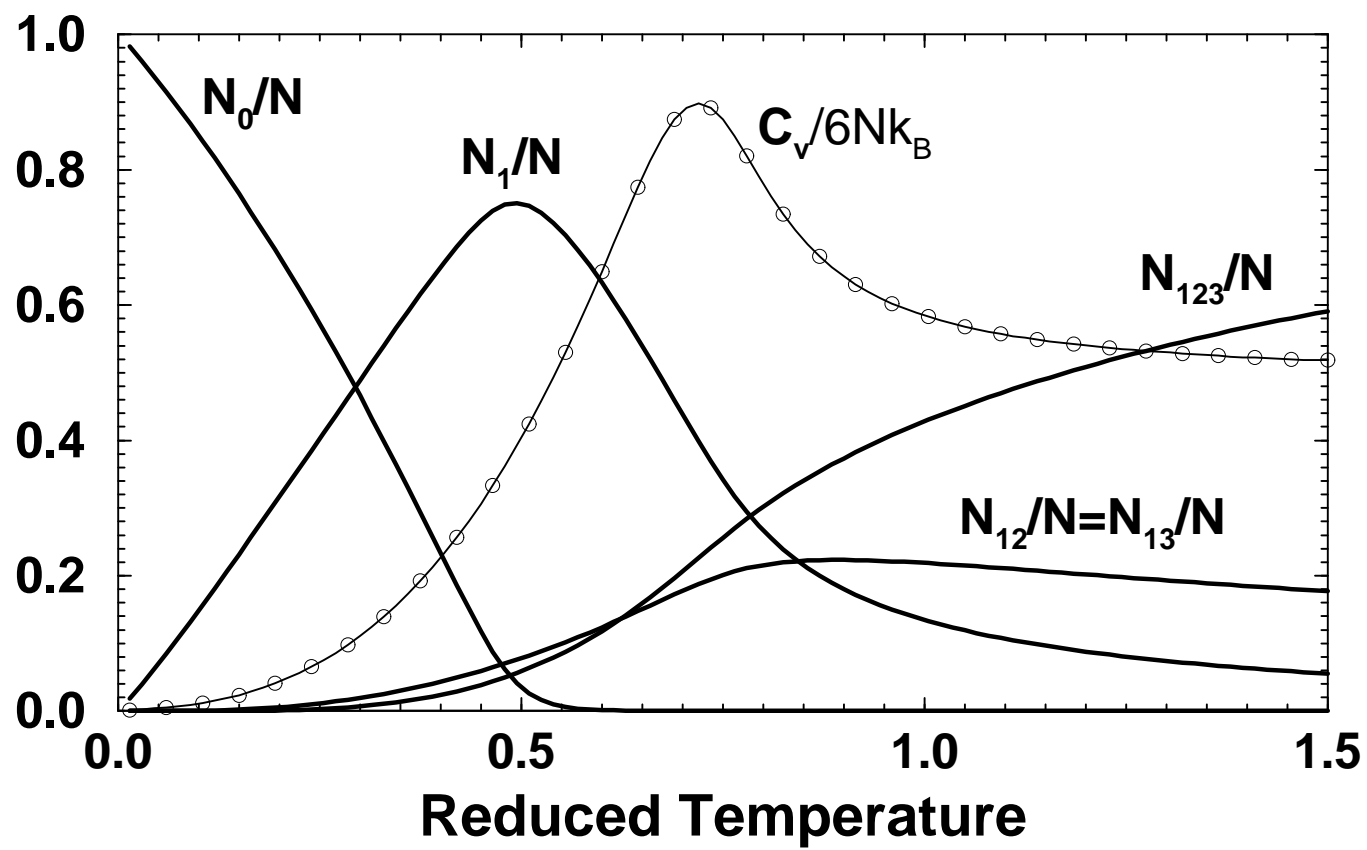


Fig.3 Wenji DENG